1987

Quantum Spin Chains: Simple Models with Complex Dynamics

Gerhard Müller
University of Rhode Island, gmuller@uri.edu

Citation/Publisher Attribution
G. Müller. *Quantum spin chains: simple models with complex dynamics.* Z. Phys. B **68** (1987), 149-159.
Available at: http://link.springer.com/article/10.1007/BF01304220

Quantum Spin Chains: Simple Models with Complex Dynamics

Gerhard Müller

Department of Physics, University of Rhode Island, Kingston RI 02881, USA

Dedicated to Professor Harry Thomas on the occasion of his 60th birthday

The present study highlights some of the complexities observed in the dynamical properties of one-dimensional quantum spin systems. Exact results for zero-temperature dynamic correlation functions are presented for two contrasting situations: (i) a system with a fully ordered ferromagnetic ground state; (ii) a system at a $T_c = 0$ critical point. For both situations it is found that the exact results are considerably more complex than has been anticipated on the basis of approximate approaches which are considered to be appropriate and reliable for such situations. A still higher degree of complexity is expected for the dynamics of quantum spin systems which are nonintegrable. The paper concludes with some observations concerning nonintegrability effects and quantum chaos in spin systems.

1. Introduction

Quantum spin chains with short-range interaction are strongly fluctuating statistical systems at all temperatures. Any spontaneous magnetic long-range order (LRO) is destabilized by thermal fluctuations at all nonzero temperatures. Even at $T = 0$, the order parameter is in general considerably reduced due to the presence of quantum fluctuations. In some cases, the quantum fluctuations prevent the onset of magnetic ordering entirely.

Quantum spin chains continue to surprise us with new unexpected features in their $T_c = 0$ critical behavior and $T = 0$ phase transitions as functions of various parameters (exchange or single-site anisotropy, magnetic field). One outstanding example has been Haldane's [1] challenging prediction that the one-dimensional (1D) spin-s Heisenberg antiferromagnet has a gap in the excitation spectrum for integer s but no gap for half-integer s, a prediction which has gained substantial support from numerical calculations even though a rigorous proof of the gap does not appear to be within reach. Moreover, some of the theoretical studies concerned with the verification and clarification of Haldane's prediction have uncovered new puzzleswhich call for further investigations (see Sect. 6 below).

For a number of cases, the $T = 0$ phase transitions of quantum spin chains map onto phase transitions of certain 2D classical statistical models in which the variable parameter is the temperature and in which the role of quantum fluctuations is taken over by thermal fluctuations. One such mapping will be discussed in Sect. 3.

Perhaps the most fascinating aspect of quantum spin chains is its dynamics. Even the most simple 1D quantum spin models turn out to reveal a degree of complexity in their dynamical properties which is hardly describable in the language of the approximation techniques commonly employed and which is frequently ignored in the interpretation of experimental measurements. Quantum spin chains are, in fact, physically realized in quasi-1D magnetic insulators for a large variety of simple models [2, 3]. Typically these are compounds in which the magnetic ions are arranged in chains along one crystallographic axis such that the exchange interaction between ions within a chain is very much stronger than the interaction between ions belonging to different chains. Two of the most important experimental techniques which probe dynamical properties of quasi-1D magnetic insulators very directly and their connection to dynamic two-spin correlation functions are the following:

(i) The inelastic scattering cross section for magnetic scattering of neutrons is directly proportional to the dynamic structure factor [2]:

$$\frac{d^2\sigma}{d\Omega d\omega} \propto S_{\mu\mu}(q,\omega) = \sum_{n=-\infty}^{+\infty} e^{-iqn} \int_{-\infty}^{+\infty} dt\, e^{i\omega t} \langle S_l^\mu(t) S_{l+n}^\mu \rangle. \tag{1.1}$$

(ii) In situations where a hydrogen ion is crystallographically located suitably close to the (electron) spin chain, the NMR spin-lattice relaxation rate $1/T_1$ of that proton is dominated by the local fluctuations of the unpaired electrons of the nearest magnetic ion [4]. It is proportional to the frequency-dependent autocorrelation function at the nuclear Larmor frequency ω_N:

$$\frac{1}{T_1} \propto \Phi_0^{\mu\mu}(\omega_N) = \int_{-\infty}^{+\infty} dt\, e^{i\omega_N t} \langle S_l^\mu(t) S_l^\mu \rangle. \tag{1.2}$$

Finally, I should like to mention Anderson's [5] proposition that magnetic singlet states of the type realized in the 1D Heisenberg antiferromagnet might be the correct starting point for a theory of the high-temperature superconductivity recently discovered in doped lanthanum copper oxides.

2. Zero-Point Fluctuations

For the purpose of illustrating the role of zero-point fluctuations in quantum spin dynamics let us consider two typical situations.

(i) The 1D Heisenberg ferromagnet (FM)

$$H_{FM} = -J \sum_{l=1}^{N} \mathbf{S}_l \cdot \mathbf{S}_{l+1} \tag{2.1}$$

has a fully ordered FM ground state $\uparrow\uparrow\uparrow \cdots \uparrow\uparrow$ irrespective of whether the spins are treated classically or quantum mechanically. It is a state without correlated fluctuations. Furthermore, the FM spin waves with dispersion $\omega_{FM}(q) = 2sJ(1-\cos q)$ are genuine small-amplitude solutions of the classical equations of motion [6] as well as exact eigenstates of the quantum Hamiltonian H_{FM} for arbitrary s. In both cases, the implication is that the $T=0$ dynamic structure factor has a sharp peak at the spin-wave frequency:

$$S_{\mu\mu}(q.\omega) = \pi s \delta\big(\omega - \omega_{FM}(q)\big) \tag{2.2}$$

where μ labels any spin component perpendicular to the order parameter.

(ii) In the case of the 1D Heisenberg antiferromagnet (AFM)

$$H_{AFM} = J \sum_{l=1}^{N} \mathbf{S}_l \cdot \mathbf{S}_{l+1} \tag{2.3}$$

the fully ordered Néel state $\uparrow\downarrow\uparrow \cdots \uparrow\downarrow$ is the ground state for classical spins but not even an eigenstate of H_{AFM} for quantum spins.

For $s = 1/2$, the true ground state of H_{AFM} is a $T_c = 0$ critical point characterized by an algebraically decaying two-spin correlation function [7]: $\langle \mathbf{S}_l \cdot \mathbf{S}_{l+n} \rangle \sim (-1)^n/n$. For $s = 1$, by contrast, the true ground state is predicted to be a nonmagnetic singlet characterized by an exponentially decaying two-spin correlation function [1]: $\langle \mathbf{S}_l \cdot \mathbf{S}_{l+n} \rangle \sim n^{-1/2} e^{-n/\xi}$. In both cases, zero-point fluctuations are responsible for a dramatic alteration of the ground state with respect to the classical Néel state. The AFM spin-waves with dispersions $\omega_{AFM}(q) = 2sJ|\sin q|$ are genuine small-amplitude solutions of the classical equations of motion [6], but there are no eigenstates of the quantum Hamiltonian H_{AFM} which could be justifiably called AFM spin waves [8]. As a direct consequence of these properties, the dynamic structure factors $S_{\mu\mu}(q,\omega)$ are much more complex than in the FM case.

For the spin-l/2 Heisenberg AFM chain, $S_{\mu\mu}(q,\omega)$ is dominated, for fixed wave number q, by a continuum of excitations rather than by a single spin-wave mode. The spectrum of these dominant excitations has been determined exactly by means of the Bethe ansatz, but the function $S_{\mu\mu}(q,\omega)$ has so far eluded any exact determination [8-10]. No detailed properties of $S_{\mu\mu}(q,\omega)$ are known for the spin-1 chain, which is not amenable to the Bethe ansatz, but AFM spin-waves are certainly a very poor representation of the true excitation spectrum. Nevertheless, it is expected that for increasing s, the complex structure of$S_{\mu\mu}(q,\omega)$ gradually gives way to an increasingly sharp peak at the AFM spin-wave frequency as the quantum fluctuations become weaker and, finally, die out in the classical limit [10]. The classical spin-wave analysis yields the following expression for the dynamic structure factor [11]:

$$S_{\mu\mu}(q,\omega) = \pi s \tan\frac{q}{2}\delta\big(\omega - \omega_{AFM}(q)\big). \tag{2.4}$$

In summary, the two situations discussed previously strongly suggest that there is, not too surprisingly, a correlation between the degree of ordering in the ground state and the degree of complexity in the $T = 0$ dynamic structure factor. Specifically, in the presence of saturated magnetic LRO, which is realized in H_{FM} for all s and in H_{AFM} for $s \to \infty$ only, $S_{\mu\mu}(q,\omega)$ has a very simple structure characterized by a δ-function at the spin-wave frequency. These observations have contributed substantially but misleadingly to the nearly all-embracing confidence in the results of the linear spin-wave analysis for 3D FM and AFM systems, where the magnetic ordering is always very strong at low temperatures except in the presence of competing interactions. The fact is that the reliability of the results obtained from the linear spin-wave analysis is by no means guaranteed by a sufficiently complete magnetic ordering in the system, i.e. by a sufficiently small amount of (quantum or thermal) fluctuations in the state of the system. It can indeed be demonstrated by rigorous calculations (see Sect. 4) that even in the presence of a fully ordered (ferromagnetic or spin flop) state the dynamic structure factors $S_{\mu\mu}(q,\omega)$ can assume a nontrivial structure, which differs dramatically from the expression produced by the linear spin-wave analysis [12, 13].

3. The Anisotropic XY Model

In the following I shall present a comparative study of the complexities observed in dynamic correlation functions of a 1D quantum spin system at $T = 0$ for two contrasting situations: (i) a situation in which the model has a fully ordered ferromagnetic ground state; (ii) a situation in which the model has a disordered ground state corresponding to a $T_c = 0$ critical point. All the results presented for these two situations are based on exact calculations for special cases of the 1D $s = 1/2$ anisotropic XY model

$$H_{AXY} = -\sum_{l=1}^{N}\big\{(1+\gamma)S_l^x S_{l+1}^x + (1-\gamma)S_l^y S_{l+1}^y + hS_l^z\big\}. \tag{3.1}$$

The 2D parameter space spanned by the exchange anisotropy γ and the magnetic field h is shown in Fig. 1.

For nonzero exchange anisotropy ($0 < \gamma \leq 1$) and subcritical fields ($0 \leq h < h_c$), the ground state of $H_{AXY}$is ferromagnetically ordered. The order parameter is the spontaneous magnetization $\bar{M}_x = \langle S_l^x\rangle$ perpendicular to the external field. Its magnitude as a function of h is [14]

$$\bar{M}_x^2 = \frac{\sqrt{\gamma}}{2(1+\gamma)}(1-h^2)^{1/4}. \tag{3.2}$$

As the field crosses the critical value $h_c = 1$, the system undergoes a continuous transition to a phase with $\bar{M}_x = 0$. In the isotropic case, on the other hand, every point on the line $0 \leq h \leq h_c$ is a critical point characterized by algebraically decaying correlation functions $\langle S_l^\mu S_{l+n}^\mu\rangle, \mu = x, y, z$.

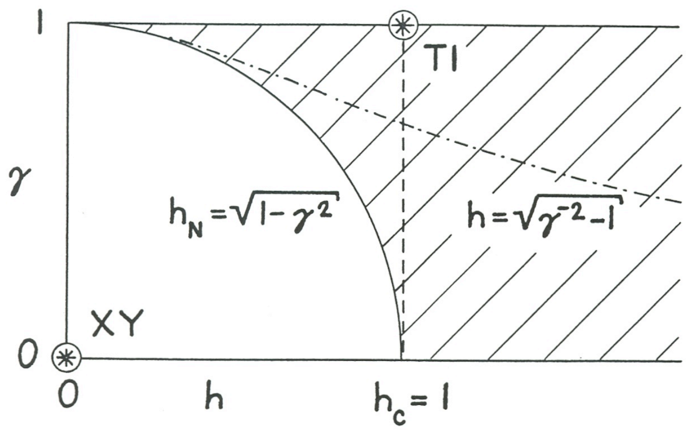

Figure 1. Two-dimensional parameter space (h, γ) of the 1D $s = 1/2$ anisotropic XY model. The shaded area denotes the region in which the ground-state properties of this model map onto the thermodynamic properties of the 2D Ising model on a rectangular lattice. In the mapping the line $h = h_N$ corresponds to $T = 0$ and $h = h_c$ to $T = T_c$. The dot-dashed line $h = \sqrt{\gamma^{-2} - 1}$ maps onto the temperature axis of the square-lattice Ising model ($J_1 = J_2$).

It is interesting to note that the ground state properties of this model in the shaded region of the parameter space shown in Fig. 1 are related, via Suzuki's mapping [15], to the thermodynamic properties of the 2D Ising model on a rectangular lattice,

$$H_I = -J_1 \sum_{n,m} \sigma_{n,m}\sigma_{n+1,m} - J_2 \sum_{n,m} \sigma_{n,m}\sigma_{n,m+1}, \tag{3.3}$$

where the coupling constants J_1, J_2 and the temperature T are determined in terms of the parameters γ, h through the relations

$$\tanh \frac{2J_1}{k_B T} = \gamma, \quad \tanh \frac{2J_2}{k_B T} = \frac{h}{h_N}. \tag{3.4}$$

In this mapping, the special field $h_N = \sqrt{1 - \gamma^2}$ of the quantum spin chain (circular line) corresponds to $T = 0$ in the 2D Ising model, whereas the critical field $h_c = 1$ (dashed line) maps onto the critical temperature T_c determined by the equation

$$\sinh \frac{2J_1}{k_B T_c} \sinh \frac{2J_2}{k_B T_c} = 1. \tag{3.5}$$

Note that the square-lattice Ising model ($J_1 = J_2$) maps onto the line $h = \sqrt{\gamma^{-2} - 1}$ in the parameter space of the anisotropic XY model (shown dot-dashed in Fig. 1).

The two-spin correlation functions of the two models H_I and H_{AXY} are related to one another as follows [15]:

$$\langle \sigma_{n,m}\sigma_{n,m'} \rangle = 2\frac{1+\gamma}{\gamma} \langle S_m^x S_{m'}^x \rangle - 2\frac{1-\gamma}{\gamma} \langle S_m^y S_{m'}^y \rangle. \tag{3.6}$$

In the limit $|m - m'| \to \infty$, this equation establishes the equivalence between the result (3.2) of Barouch and McCoy [14] for the order parameter of the 1D anisotropic XY model and the Onsager-Yang result for the spontaneous magnetization of the 2D Ising model [16]:

$$\bar{M}^2 = 2\frac{1+\gamma}{\gamma} \bar{M}_x^2 = \left\{ 1 - \mathrm{cosech}\frac{2J_1}{k_B T} \mathrm{cosech}\frac{2J_2}{k_B T} \right\}^{1/4}. \tag{3.7}$$

Furthermore, Suzuki's mapping establishes the equivalence between the logarithmic divergence of the susceptibility $\bar{\chi}_{zz}(T = 0, h) = \partial \bar{M}_z / \partial h$ at $h = h_c$ of the 1D quantum spin model H_{AXY}

and the logarithmic divergence of the specific heat at $T = T_c$ of the 2D Ising model. Thus the magnetization $\bar{M}_z$, which is not the order parameter of the $T = 0$ phase transition in the quantum spin chain, plays a role analogous to the entropy in the 2D Ising model and the quantity $h\bar{\chi}_{zz}$ a role analogous to the specific heat. The divergence of the 2D Ising model susceptibility $\chi(T) \sim |T - T_c|^{-7/4}$, on the other hand, has its equivalence in an analogous singularity of the susceptibility $\bar{\chi}_{xx}(T = 0, h) \sim |h - h_c|^{-7/4}$ of the 1D quantum spin model.

Returning to the comparative study of dynamic correlation functions, we recall the well-known fact that the $s = 1/2$ anisotropic XY model (3.1) maps, via the Jordan-Wigner transformation

$$\begin{aligned} S_l^+ &= S_l^x + \mathrm{i}S_l^y = a_l^\dagger \exp\left(\mathrm{i}\pi \sum_{j<l} a_j^\dagger a_j\right) \\ S_l^- &= S_l^x - \mathrm{i}S_l^y = \exp\left(-\mathrm{i}\pi \sum_{j<l} a_j^\dagger a_j\right) a_l \\ S_l^z &= a_l^\dagger a_l - \frac{1}{2} \end{aligned} \tag{3.8}$$

onto a system of noninteracting fermions with the following one-particle spectrum [17, 18] :

$$\omega_k = \mathrm{sgn}(h + \cos k)\sqrt{(h + \cos k)^2 + \gamma^2 \sin^2 k}. \tag{3.9}$$

As a result of the simple structure of the operator S_l^z in the fermion representation, the dynamic structure factor $S_{zz}(q, \omega)$ can be expressed in terms of a fermion density-density correlation function, i.e. in terms of a 2-particle Green's function, which can be evaluated under all circumstances [19, 20]. The dynamic structure factors $S_{xx}(q, \omega)$ and $S_{yy}(q, \omega)$, on the other hand, have a much more complicated structure in the fermion representation, caused by the exponential operators in the Jordan-Wigner transformation. These functions are expressible in terms of infinite block Töplitz determinants [21], i.e. in terms of quantities which are, in general, not readily evaluated except for very special circumstances.

The two contrasting situations (i) and (ii), mentioned at the beginning of this section, can now be identified as follows: Situation (i) is realized along the circular line $h = h_N = \sqrt{1 - \gamma^2}$, $0 \le \gamma \le 1$ (see Fig. 1) where the system has a ferromagnetic ground state characterized by the order parameter

$$\mathbf{M} = \langle \mathbf{S}_l \rangle = \frac{1}{2}\Big(\sqrt{2\gamma/(1+\gamma)}, 0, \sqrt{(1-\gamma)(1+\gamma)}\Big). \tag{3.10}$$

Situation (ii) is realized (not exclusively) at the following two points (marked by asterisks in Fig. 1): (a) $h = \gamma = 1$. This is the transverse Ising (TI) model at the critical field. Its equal-time two-spin correlation functions decay algebraically as follows [14] :

$$\langle S_l^x S_{l+n}^x \rangle \sim n^{-1/4}, \quad \langle S_l^y S_{l+n}^y \rangle \sim n^{-9/4}, \quad \langle S_l^z S_{l+n}^z \rangle - \bar{M}_z^2 \sim n^{-2}. \tag{3.11}$$

(b) $h = \gamma = 0$. This is the isotropic XY model in zero field. Its correlation functions have the following long-distance asymptotic behavior:

$$\langle S_l^x S_{l+n}^x \rangle = \langle S_l^y S_{l+n}^y \rangle \sim n^{-1/2}, \quad \langle S_l^z S_{l+n}^z \rangle \sim n^{-2}. \tag{3.12}$$

4. Dynamics of a Quantum Spin Chain in its Fully Ordered Ferromagnetic Ground State

Here we are concerned with situation (i) as specified in the preceding Sect. However, starting out with the study of a model which is more general than the $s = 1/2$ anisotropic XY model (3.1), we may ask the question [11-13]: Under what circumstances does the general spin-s XYZ FM in a uniform magnetic field

$$H_{XYZ} = -\sum_{l=1}^{N} \left[J_x S_l^x S_{l+1}^x + J_y S_l^y S_{l+1}^y + J_z S_l^z S_{l+1}^z + h S_l^z \right] \tag{4.1}$$

for $J_x \geq J_y \geq J_z \geq 0$, even N and periodic boundary conditions have a ground state wave function of the form

$$|G\rangle = \bigotimes_{l=1}^{N} |\vartheta, l\rangle,$$
$$|\vartheta, l\rangle = U_l(\vartheta)|s\rangle_l = \sum_{m=-s}^{+s} \left[\frac{(2s)!}{(s+m)!(s-m)!} \right]^{1/2} \left[\cos\frac{\vartheta_l}{2} \right]^{s+m} \left[\sin\frac{\vartheta_l}{2} \right]^{s-m} |m\rangle_l, \tag{4.2}$$

where $U_l(\vartheta)$ describes a unitary transformation representing a rotation of the spin direction at the site l by an angle ϑ away from the z-axis in the xz-plane? $|G\rangle$ is a state of maximum magnetic order

$$\mathbf{M} = \langle \vartheta, l | \mathbf{S}_l | \vartheta, l \rangle = (s \sin\vartheta, 0, s\cos\vartheta) \tag{4.3}$$

with no correlated fluctuations. An alternative formulation of this question, which has proven to be useful for the analysis of the problem, is the following: Under what circumstances does the Hamiltonian

$$\tilde{H}_{XYZ} = U^{-1} H_{XYZ} U, \quad U = \bigotimes_{l=1}^{N} U_l(\vartheta) \tag{4.4}$$

have a ground-state wave function of the simple form

$$|\tilde{G}\rangle = U^{-1}|G\rangle = \bigotimes_{l=1}^{N} |s\rangle_l = |\uparrow\uparrow \cdots \uparrow\rangle \tag{4.5}$$

with all spins aligned parallel to the z-axis? For given values of the exchange constants $J_x \geq J_y \geq J_z$, the XYZ model (4.1) has indeed a ground state of the form (4.2) with

$$\cos\vartheta = \sqrt{(J_y - J_z)/(J_x - J_z)} \tag{4.6}$$

provided the magnetic field assumes the value

$$h = h_N = 2s\sqrt{(J_x - J_z)(J_y - J_z)}. \tag{4.7}$$

See Fig. 2 for a schematic illustration of this state. The ground-state energy is then given by

$$E_G = \langle G | H_{XYZ} | G \rangle = \langle \tilde{G} | \tilde{H}_{XYZ} | \tilde{G} \rangle = -Ns^2(J_x + J_y - J_z) \tag{4.8}$$

and the transformed Hamiltonian $\tilde{H}_{XYZ}$ whose ground-state wave function is $|\tilde{G}\rangle = |\uparrow\uparrow \cdots \uparrow\rangle$ reads [13]:

$$\begin{aligned} \tilde{H}_{XYZ} = -\sum_{l=1}^{N} \Big[& J_y (S_l^x S_{l+1}^x + S_l^y S_{l+1}^y) + (J_x - J_y + J_z) S_l^z S_{l+1}^z + 2s(J_y - J_z) S_l^z \\ & + \big\{ (J_x - J_y)(J_y - J_z) \big\}^{1/2} \big\{ S_l^z S_{l+1}^x + S_l^x S_{l+1}^z - s(S_{l+1}^x + S_l^x) \big\} \Big]. \end{aligned} \tag{4.9}$$

The circular line in Fig. 1 represents a special case of this situation.

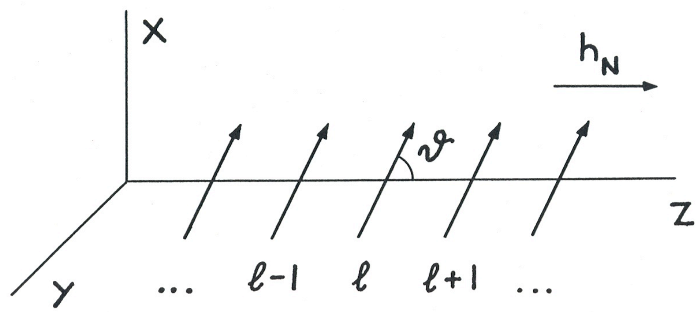

Figure 2. Schematic illustration of the direct-product ground state (4.3) of the spin-s XYZ ferromagnet H_{XYZ} with $J_x \geq J_y \geq J_z \geq 0$ in a magnetic field of magnitude $h = h_N$ parallel to the z-axis.

After having established this solution, we may ask: Under what conditions are the ferromagnetic spin wave states

$$|\tilde{q}\rangle = S_q^- |\tilde{G}\rangle, \quad S_q^- = N^{-1/2} \sum_{l=1}^{N} \mathrm{e}^{-\mathrm{i}ql} S_l^- \tag{4.10}$$

also eigenstates ofH_{XYZ}? The condition is that the second term on the right-hand side of the following equation vanishes:

$$\begin{aligned} \big[\tilde{H}_{XYZ}, S_q^-\big]|\tilde{G}\rangle &= \omega_{SW}(q) S_q^- |\tilde{G}\rangle \\ &+ \frac{1}{2}\sqrt{(J_x - J_y)(J_y - J_z)}(1 + \mathrm{e}^{-\mathrm{i}q}) N^{-1/2} \sum_l \mathrm{e}^{-\mathrm{i}ql} S_l^- S_{l+1}^- |\tilde{G}\rangle, \end{aligned} \tag{4.11}$$

where $\omega_{SW}(q) = 2s(J_x - J_y \cos q)$ is the dispersion predicted by linear spin-wave theory. Hence, linear spin waves are eigenstates of H_{XYZ} if one of the following three conditions is satisfied [13]:

(i) $J_x = J_y$; arbitrary q and s

(ii) $q = \pi$; arbitrary J_x, J_y, J_z, and s

(iii) $s \to \infty$; arbitrary J_x, J_y, J_z, and q.

Only under these additional conditions do the $T = 0$ dynamic structure factors of H_{XYZ} have zero linewidth. In all other cases, they have a nontrivial structure in spite of the very special ground-state wave function. Nevertheless, one can prove that in the presence of a product ground state $|G\rangle$ the following linear relations between the dynamic structure factors $S_{\mu\mu}(q,\omega)$, $\mu = x, y, z$ of H_{XYZ} at $T = 0$ are satisfied [13]:

$$\begin{aligned} S_{xx}(q,\omega) &= S_{yy}(q,\omega)\cos^2\vartheta + 4\pi^2 s^2 \sin^2\vartheta\,\delta(\omega)\delta(q) \\ S_{zz}(q,\omega) &= S_{yy}(q,\omega)\sin^2\vartheta + 4\pi^2 s^2 \cos^2\vartheta\,\delta(\omega)\delta(q \end{aligned} \tag{4.12}$$

with ϑ from (4,6).

In search of cases for which the nontrivial structure of the quantities $S_{\mu\mu}(q,\omega)$ for the spin-s model H_{XYZ} with FM ground state $|G\rangle$ or for the spin-s model $\tilde{H}_{XYZ}$ with FM ground state $|\tilde{G}\rangle$ can be determined exactly, we now focus the analysis onto the $s = 1/2$ anisotropic XY model $J_x = 1 + \gamma, J_y = 1 - \gamma, J_z = 0)$ at $h = h_N = \sqrt{1-\gamma^2}$. For this case we can take advantage of the fact that the function $S_{zz}(q,\omega)$ is expressible in terms of a 2-particle Green's function for free fermions and is thus readily evaluated. The exact result reads [12]

$$S_{zz}(q,\omega) = \pi^2 \frac{1-\gamma}{1+\gamma}\delta(\omega)\delta(q) + \frac{\gamma^2}{1-\gamma^2} \frac{\sqrt{4(1-\gamma^2)\cos^2(q/2)-(\omega-2)^2}}{\left[\omega - 2\sin^2(q/2)\right]^2 + \gamma^2 \sin^2 q} \Theta\left[4(1-\gamma^2)\cos^2(q/2) - (\omega-2)^2\right] \tag{4.13}$$

and is plotted in Fig. 3. It is nonzero for values of (q,ω) within the range of the two-fermion spectrum $|\omega - 2| < \cos(q/2)$ and is strikingly different from the δ-function predicted by linear spin-wave theory,

$$S_{zz}^{(SW)}(q,\omega) = \frac{\pi\gamma}{1+\gamma}\delta\big(\omega - \omega_{SW}(q)\big), \quad \omega_{SW}(q) = (1+\gamma) - (1-\gamma)\cos q \tag{4.14}$$

despite the fact that the ground state $|G\rangle$ is fully ferromagnetically ordered. In fact, the spin-wave dispersion $\omega_{SW}(q)$ differs considerably from the peak frequency of the exact result (4.13) except for $q = \pi$. It is noteworthy that the two functions $S_{xx}(q,\omega)$ and $S_{yy}(q,\omega)$, which in general have a much more complicated structure than the function $S_{zz}(q,\omega)$, differ from $S_{zz}(q,\omega)$ for this particular situation only by an overall γ-dependent factor as a result of the relations (4.12). This simplification is not at all evident in the fermion representation.

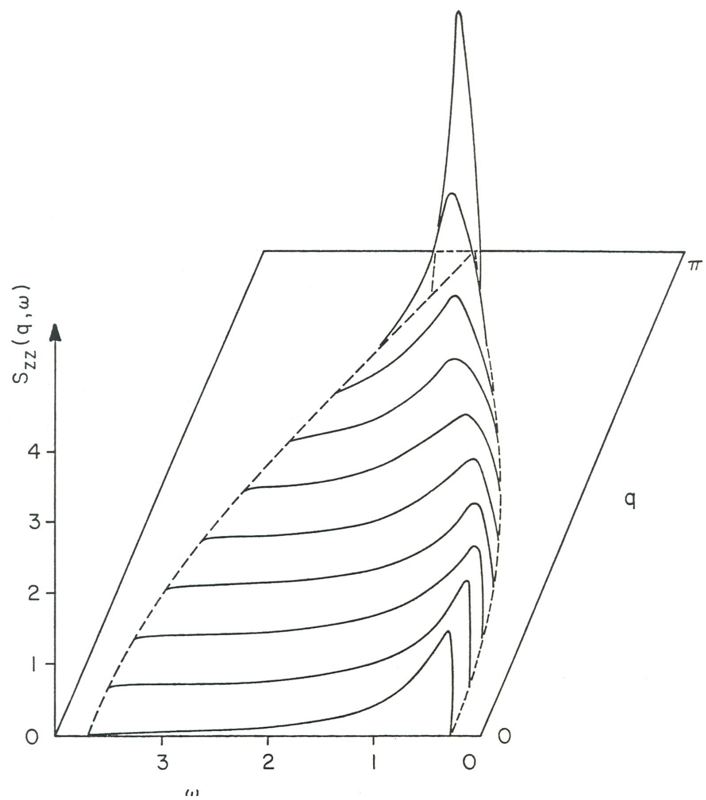

Figure 3. Dynamic structure factors $S_{zz}(q,\omega)$ as a function of frequency at wave numbers $q = n\pi/10$, $n = 0, 1, \ldots, 9$ for the 1D $s = 1/2$ anisotropic XY model (3.1) at $T = 0$ and $h = h_N = \sqrt{1-\gamma^2}$, $\gamma = 1/2$. Not shown is the δ-function contribution at $q = \omega = 0$, which represents the saturated ferromagnetic long-range order in the system.

Even though the exact result (4.13) is not readily generalizable to models with spin $s > 1/2$, it can be shown by means of exact sum rules in the form of frequency moments [12] that the linewidth of the dynamic structure factors $S_{\mu\mu}(q,\omega)$), which is appreciable for $s = 1/2$ (see Fig. 3), goes to zero gradually in the limit $s \to \infty$. These exact and explicit results thus demonstrate that even in the presence of a fully ordered FM ground state, the dynamic structure factors $S_{\mu\mu}(q,\omega)$) can exhibit a nontrivial ω-dependence and invalidate the spin-wave analysis seriously. Since this appreciable complexity of $S_{\mu\mu}(q,\omega)$) cannot be attributed to the presence of strong (quantum or thermal) fluctuations in this 1D model, there is no a priori reason to assume that similar effects should be less pronounced in 2D and 3D magnetic systems.

5. Dynamics of a Quantum Spin Chain at a $T_c = 0$ Critical Point

Here I would like to highlight some exact results for the two-spin correlation functions

$$\Xi_n(t) \equiv 4\langle S_l^\xi(t) S_{l+n}^\xi \rangle, \quad \xi = x, y, z \tag{5.1}$$

and their frequency-dependent Fourier transforms

$$\Phi_n^{\xi\xi}(\omega) = \int_{-\infty}^{+\infty} dt\, \mathrm{e}^{\mathrm{i}\omega t} \langle S_l^\xi(t) S_{l+n}^\xi \rangle \tag{5.2}$$

for the two cases (a) $h = \gamma = 1$ and (b) $h = \gamma = 0$ of the 1D $s = 1/2$ anisotropic XY model (3.1) at $T = 0$, representing the transverse Ising (TI) model at the critical field and the isotropic XY model in zero field, respectively. These two cases correspond to situation (ii) as specified at the beginning of Sect. 3.

The correlation function $Z_n(t)$ can be expressed quite generally in terms of a 2-particle Green's function for free fermions [19, 20]. Hence this function does not show any increase in complexity for situation (ii) with respect to situation (i) described in Sect. 4. This is not the case, however, for the correlation functions $X_n(t)$ and $Y_n(t)$, which are expressible, generally, in terms of infinite block Töplitz determinants [21] and thus have, in general, a much more complicated structure than in situation (i).

For the two cases of interest here they are [22]

$$\left[X_n(t)_{TI}\right]^4 = \lim_{N\to\infty} \begin{vmatrix} a_0 & a_{-1} & \cdots & a_{-N} \\ a_1 & a_0 & \cdots & a_{-N+1} \\ \vdots & \vdots & \cdots & \vdots \\ a_N & a_{N-1} & \cdots & a_0 \end{vmatrix} \tag{5.3}$$

$$a_l = \frac{1}{2\pi}\int_0^{2\pi} d\vartheta\, \mathrm{e}^{-\mathrm{i}l\vartheta} \begin{bmatrix} \tanh(\beta\sin\vartheta) & \mathrm{e}^{2\mathrm{i}n\vartheta - 2\mathrm{i}t\sin\vartheta}\left[1+\tanh(\beta\sin\vartheta)\right] \\ -\mathrm{e}^{-2\mathrm{i}n\vartheta+2\mathrm{i}t\sin\vartheta}\left[1-\tanh(\beta\sin\vartheta)\right] & \tanh(\beta\sin\vartheta) \end{bmatrix}$$

$$Y_n(t)_{TI} = -\frac{d^2}{dt^2} X_n(t)_{TI} \tag{5.4}$$

$$X_n(t)_{XY} = Y_n(t)_{XY} = \begin{cases} \left[X_{n/2}(t/2)_{TI}\right]^2, & n \text{ even} \\ X_{(n-1)/2}(t/2)_{TI} X_{(n+1)/2}(t/2)_{TI}, & n \text{ odd} \end{cases} \tag{5.5}$$

where $\beta = 1/k_B T$.

It was a major accomplishment in quantum spin dynamics to transform expression (5.3) for $T = 0$ into the form [22]

$$X_n(t)_{TI} = X_n(0)_{TI} \exp\left(-\frac{1}{2}t^2 + \int_0^{2t} dt' \frac{\sigma_n(\mathrm{i}t')}{t'}\right), \tag{5.6}$$

where $X_n(t)_{TI}$ is the known equal-time correlation function and $\sigma_n(z)$ satisfies the nonlinear ordinary differential equation (ODE)

$$\left(z\sigma_n''\right)^2 + 4\left[z\sigma_n' - \sigma_n - n^2\right]\left[z\sigma_n' - \sigma_n + \left(\sigma_n'\right)^2\right] = 0 \tag{5.7}$$

for specific initial conditions. The analysis of this solution has revealed a degree of complexity in the structure of time-dependent correlation functions $\Xi_n(t)_{TI}$ and $\Xi_n(t)_{XY}$, $\xi = x, y, z$ not previously observed in quantum spin systems. It is well documented in Refs. [22, 23]. However, the most important features of these functions are best visualized in their frequency-dependent Fourier transforms, which have been determined by high-precision numerical calculations combined with an exact analysis of their singularity structure [23]. The $T = 0$ frequency-dependent autocorrelation functions $\Phi_0^{\xi\xi}(\omega)_{TI}$ and $\Phi_0^{\xi\xi}(\omega)_{XY}$, $\xi = x, y, z$ are shown in Figs. 4 and 5, respectively. The characteristic properties of these functions, which are likely to reflect many generic features of the dynamical properties of integrable quantum many-body systems, may be summarized as follows:

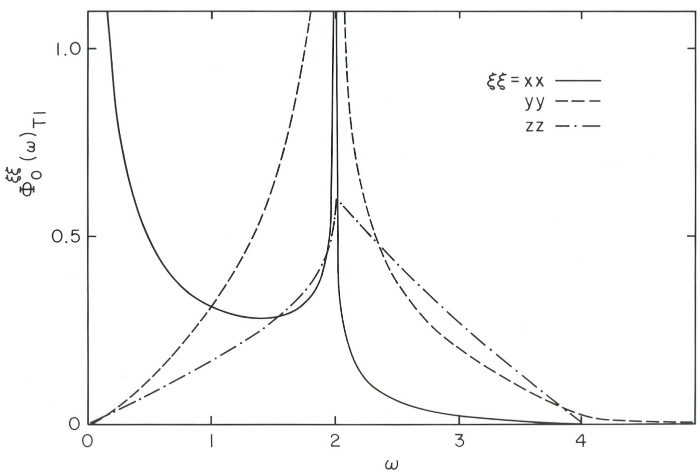

Figure 4. Frequency-dependent autocorrelation functions $\Phi_0^{xx}(\omega)_{TI}$ (solid line), $\Phi_0^{yy}(\omega)_{TI}$ (dashed line), and $\Phi_0^{zz}(\omega)_{TI}$ (dot-dashed line) for the 1D $s = 1/2$ transverse Ising model at the critical field and $T = 0$.

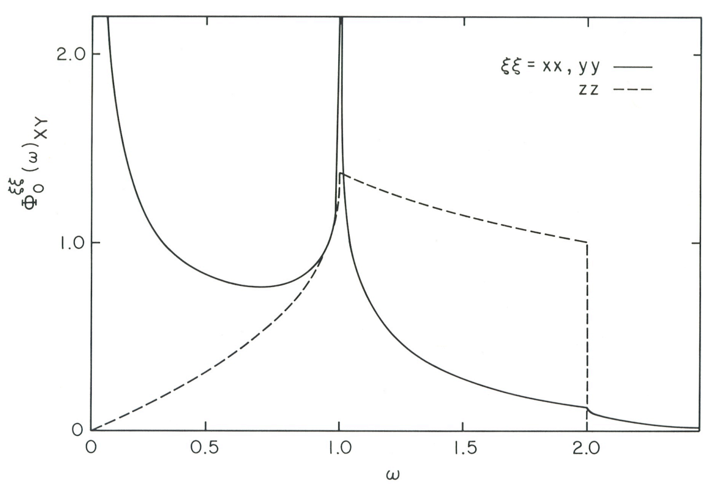

Figure 5. Frequency-dependent autocorrelation functions $\Phi_0^{xx}(\omega)_{XY} = \Phi_0^{yy}(\omega)_{XY}$ (solid line) and $\Phi_0^{zz}(\omega)_{XY}$ (dashed line) for the 1D $s = 1/2$ XY model in zero field and at $T = 0$.

(i) The functions $\Phi_0^{xx}(\omega)_{TI}$, $\Phi_0^{yy}(\omega)_{TI} = \omega^2\Phi_0^{xx}(\omega)_{TI}$ and $\Phi_0^{xx}(\omega)_{XY} = \Phi_0^{yy}(\omega)_{XY}$ have nonzero spectral weight for arbitrarily high frequencies, whereas the functions $\Phi_0^{zz}(\omega)_{TI}$ and $\Phi_0^{zz}(\omega)_{XY}$ are of compact support.

(ii) The function $\Phi_0^{xx}(\omega)_{TI}$ has an infinite set of singularities at frequencies $\omega = 2m$, $m = 0, 1, 2, \ldots$ of the form [23]:

$$\Phi_0^{xx}(\omega)_{TI}^{(m)} \sim \frac{1}{2} A_m \Gamma\left(\frac{3}{4} - \frac{1}{2}m^2\right) |\omega - 2m|^{\nu_m^{(TI)}} \left\{\frac{1}{2}\left[1 - (-1)^m\right]\Theta(2m - \omega) + 2^{-1/2}\Theta(\omega - 2m)\right\} \tag{5.8}$$

where

$$A_m = \bar{A}(2\pi)^{-m/2} 2^{-m^2/2} a_m, \quad \bar{A} = 2^{1/12} \exp\left(3\zeta'(-1)\right),$$

$\nu_m^{(TI)} = m^2/2 - 3/4$, $\zeta(z)$ is the Riemann zeta function, and the coefficients a_m are positive rational numbers. These power-law singularities are one-sided for even m and two-sided for odd m. Only the first two singularities ($m = 0, 1$) are divergent: $\sim \omega^{-3/4}\Theta(\omega)$ at $\omega \simeq 0$ and $|\omega - 2|^{-1/4}[\Theta(2 - \omega) + 2^{-1/2}\Theta(\omega - 2)]$ at $\omega \simeq 2$. In the function $\Phi_0^{yy}(\omega)_{TI}$ the divergence at $\omega = 0$ is suppressed by the factor ω^2 which relates it to $\Phi_0^{xx}(\omega)_{TI}$. Note that only 3 (nondivergent) singularities occur in $\Phi_0^{zz}(\omega)_{TI}$, which is identically zero for $\omega \geq 4$.

(iii) Similarly, the functions $\Phi_0^{xx}(\omega)_{XY} = \Phi_0^{yy}(\omega)_{XY}$ are characterized by an infinite set of singularities at frequencies$\omega = m$, $m = 0, 1, 2, \ldots$ These singularities are alternatingly one-sided power-type (m even) and two-sided power-type with logarithmic corrections (m odd) [23]:

$$\Phi_0^{xx}(\omega)_{XY}^{(m)} \sim \begin{cases} \frac{1}{2} B_m \Gamma\left(\frac{1}{2} - \frac{1}{4}m^2\right) (\omega - m)^{\nu_m^{(XY)}} \Theta(\omega - m), & \text{even } m \\ -\frac{1}{2} B_m \left\{\left[\frac{1}{4}(m^2 - 1)\right]!\right\}^{-1} |\omega - m|^{\nu_m^{(XY)}} \ln|\omega - m|, & \text{odd } m \end{cases} \tag{5.9}$$

where $B_m = \bar{A}^2\sqrt{2}(2\pi)^{-m/2} b_m$, $\nu_m^{(XY)} = \frac{1}{4}(m^2 - 2)$ for even m and $\nu_m^{(XY)} = \frac{1}{4}(m^2 - 1)$ for odd m; the coefficients b_m are positive rational numbers. In particular, the singularities visible in Fig. 5 are the two divergences $\sim \omega^{-1/2}\Theta(\omega)$ at $\omega = 0$, $\sim \ln|\omega - 1|$ at $\omega = 1$, and the cusp $\sim (\omega - 2)^{1/2}\Theta(\omega - 2)$ at $\omega = 2$. The function $\Phi_0^{zz}(\omega)_{XY}$ again has only 3 singularities and vanishes for $\omega > 2$.

(iv) The regular patterns of singularities in $\Phi_0^{xx}(\omega)_{TI}$ and $\Phi_0^{xx}(\omega)_{XY}$ are attributable to the fact that the excitation spectrum of these functions can be decomposed (in the fermion representation) into sets of m-particle excitations with energies

$$\epsilon_m(k_1, k_2, \ldots, k_m) = \sum_{l=1}^{m} |\omega_{k_i}|, \quad q = \sum_{l=1}^{m} k_i \tag{5.10}$$

for arbitrarily large m, whose densities of states have van Hove singularities at exactly the frequencies $\omega = 2m$ (TI) or $\omega = m$ (XY), $m = 0, 1, 2, \ldots$ This illustrates the fact that the functions $\Phi_0^{xx}(\omega)_{TI}$ and $\Phi_0^{xx}(\omega)_{XY}$ couple to the m-particle spectrum for arbitrarily large m in contrast to the functions $\Phi_0^{zz}(\omega)_{TI}$ and $\Phi_0^{zz}(\omega)_{XY}$ which couple only to the 2-particle excitations characterized by just 3 van Hove singularities [21, 23]. It is important to point out in this context that the exact nature (exponent, amplitude) of the singularities as they appear in these functions is governed, in general, by the effects of matrix elements and not by the densities of states alone.

(v) On the intervals between the singularities, the autocorrelation functions of both the TI and the XY models are convex functions of ω: $(d^2/d\omega^2)\Phi_0^{\mu\mu}(\omega) > 0$, $\mu = x, y, z$. Hence these functions have no smooth maxima; all maxima occur at points of nonanalyticity. Even though the functions $\Phi_0^{xx}(\omega)_{TI}$ and $\Phi_0^{xx}(\omega)_{XY}$ have spectral weight at arbitrarily high frequencies, they approach zero at least as rapidly as $\sim \exp(-a\omega^2)$ for $\omega \to \infty$, where a is a positive constant [23].

(vi) The Luttinger model is understood to represent a continuum version of the 1D $s = 1/2$ XXZ model, which contains the isotropic XY model as a special case, namely that of free fermions. The calculation of the function $\Phi_0^{xx}(\omega)_{XY}$ for the Luttinger model [7] yields the correct exponents for the leading and next-leading singularities at $\omega = 0$ as given in (5.9). However, it fails to reproduce any of the nonanalyticities at $\omega > 0$. This is not surprising in view of the fact that these singularities are intrinsic features of the discrete quantum spin system and cannot be accounted for by a continuum analysis.

(vii) It is interesting to note that the correlation functions $\Phi_0^{xx}(\omega)_{XY}$ and $\Phi_0^{yy}(\omega)_{XY}$ can, in fact, also be expressed in terms of 2-particle Green's functions, but for *interacting* fermions as opposed to noninteracting fermions in the case of $\Phi_0^{zz}(\omega)_{XY}$. This representation is obtained simply by means of a coordinate transformation in spin space preceding the Jordan-Wigner transformation. The coupling of the functions Φ_0^{xx} and Φ_0^{yy} to the m-particle excitations for $m > 2$ and arbitrarily large can then be understood as being caused by the infinite hierarchy of m-particle Green's functions generated in the equation of motion for the 2-particle Green's function by the interaction term of the fermion Hamiltonian.

6. Effects of Nonintegrability and Quantum Chaos

Notwithstanding the high degree of complexity observable in the dynamical properties of quantum spin chains as demonstrated by exact results in the preceding two sections, we have to bear in mind that this type of rigorous analysis is strictly limited to integrable models. In studying the dynamical properties of quantum spin models which are intrinsically *nonintegrable* (as the majority of realistic models probably are), it would be naive not to be prepared for the encounter of new levels of complexity.

It is well known that the role of integrability is quite striking in the behavior of classical dynamical systems. The dynamical properties of integrable systems are observed to undergo dramatic changes if subjected to nonintegrable perturbations, producing qualitatively new phenomena. These phenomena are manifestations of deterministic chaos and have been the object of extensive studies [24]. This raises a question of considerable interest: What are the implications of integrability and nonintegrability for quantum many-body systems in general and for quantum spin chains in particular, and how are these implications related to the important and still unresolved issue of quantum chaos? A recent study of the nature of quantum chaos [25] in spin systems has put the concepts of integrability for classical and quantum spin systems into perspective and has outlined the similarities and differences between effects of nonintegrability in the two cases (see also Ref. 26). The focus of the following remarks are nonintegrability effects in quantum spin chains and their interpretation as manifestations of quantum chaos.

Chaotic phenomena in quantum many-body systems are expected to be most dramatically apparent in dynamical correlation functions. Hence, one might wish to study primarily the dynamical properties of quantum spin chains. The problem is that dynamical properties of such systems are, in general, highly nontrivial and therefore difficult to analyze even for integrable models. This makes it very difficult to identify nonintegrability effects there. Nevertheless, a scrutinizing study of the dynamical properties of integrable quantum many-body systems is likely to provide the clue for specific characteristic features which result as a consequence of integrability and whose absence amounts to the relaxation of certain constraints. This strategy has been very successful in the study of classical Hamiltonian chaos: the foliation of the entire phase space by invariant tori is a consequence of integrability, and the presence of chaotic trajectories implies that this pattern is at least partially destroyed [24, 26].

A property of dynamic correlation functions for infinite quantum spin systems which is likely to be very sensitive to the integrability and nonintegrability of the underlying model is the general structure of the excitation spectrum. Characteristic for all quantum spin models which are integrable in the thermodynamic limit, by means of the Bethe ansatz or related techniques, is that the entire excitation spectrum is composed of multiparameter continua, i.e. structures with well-defined boundaries, which give rise to power-law or logarithmic van Hove singularities in the corresponding densities of states. These singularities are bound to make their appearance also in dynamical properties, specifically in frequency-dependent correlation functions for pure quantum states,

$$\Phi_n^{\mu\mu}(\omega) = \int_{-\infty}^{+\infty} dt\, \mathrm{e}^{\mathrm{i}\omega t} \langle\psi|\mathrm{e}^{\mathrm{i}Ht} S_l^\mu \mathrm{e}^{-\mathrm{i}Ht} S_{l+n}^\mu|\psi\rangle. \tag{6.1}$$

If this is the case, they impose the constraint that the corresponding time-dependent correlation functions $\langle\psi|S_l^\mu(t)S_{l+n}^\mu|\psi\rangle$ cannot decay faster than by powers of t asymptotically for $t \to \infty$.

This peculiar property is very well documented for the case of the 1D $s = 1/2$ anisotropic XY model (3.1) some of whose $T = 0$ dynamical properties have been discussed in Secs. 4 and

5. For this model, it was shown that the zero-temperature time-dependent two-spin correlation functions $\langle S_l^\mu(t)S_{l+n}^\mu\rangle$ decay (for fixed n) by powers of t to their long-time asymptotic values irrespective of whether the corresponding equal-time correlation functions $\langle S_l^\mu S_{l+n}^\mu\rangle$ decay to their long-distance ($n\to\infty$) asymptotic values exponentially or algebraically [21]. In fact, the constraint that time-dependent two-spin correlation functions for pure quantum states $\langle\psi|S_l^\mu(t)S_{l+n}^\mu|\psi\rangle$ do not decay faster than algebraically to their long-time asymptotic values appears to be a universal feature of integrable quantum spin systems in the thermodynamic limit, in consequence of the property that the entire excitation continuum of such systems has a multi-parameter continuum structure. This constraint is paralleled in integrable classical dynamical systems with N degrees of freedom by the universal property that each individual phase-space trajectory is confined to an N-dimensional hypersurface, in consequence of the complete foliation of the $2N$-dimensional phase space by invariant tori. In both cases the constraint is the result of the existence of a sufficient number of conservation laws.

These observations on integrable quantum spin models strongly suggest that a characteristic property of *nonintegrable* quantum spin models might be that there exist pure quantum states $|\psi\rangle$ for which the time-dependent correlation functions $\langle\psi|S_l^\mu(t)S_{l+n}^\mu|\psi\rangle$ decay more rapidly to their asymptotic values than by powers of t [25]. Incidentally, exponentially decaying time-correlation functions are characteristic for special classes of nonintegrable classical dynamical systems with few degrees of freedom [27].

One immediate and far-reaching consequence of rapidly decaying spin correlation functions $\langle\psi|S_l^\mu(t)S_{l+n}^\mu|\psi\rangle$ would be the presence of excitations with unusual spectral properties. Nonintegrable quantum spin systems would then possess two types of spectrum, the *regular* and the *irregular* spectrum. Again, this is paralleled by the occurrence of two types of spectrum in classical dynamical systems: the discrete spectrum of *regular* trajectories and the continuous spectrum of *chaotic* trajectories. In quantum spin systems, the *regular* part of the spectrum consists of multi-parameter continua, and is characterized by the property that for an increasing number N of spins, individual excitations belonging to a particular continuum close up as $1/N$ in $(\mathbf{q},\omega)$-space to an increasingly regular pattern. Hence it is the regular multi-parameter continuum structure of the spectrum rather than its discreteness which is the hallmark of a quantum invariant torus. The *irregular* part of the spectrum consists of excitations which do not form regular patterns. The absence of individual branches or continua with well-defined boundaries, which would invariably lead to van Hove singularities, must be the result of strong level repulsion, attributable to the nonexistence of a sufficient number of conservation laws (expressible in terms of a complete set of quantum numbers). It is highly suggestive to view in the irregular spectrum a manifestation of quantum chaos [25].

Naturally, the study of quantum chaos as portrayed in this paper is limited for the most part to the study of its precursors in finite-N systems of nonintegrable quantum many-body models. Nonintegrability effects in quantum spin chains of finite size (finite N) are expected to make their appearance in the form of an intensifying level turbulence for increasing N, which would manifest itself, for example, in the form of changes in trend in $1/N$ extrapolations, in the failure of expected scaling behavior, and in the presence of unusual classes of excitations. In integrable quantum spin models, the characteristic excitation pattern of the infinite system is apparent even in relatively short chains. This is generally not the case in nonintegrable models. Here, finite-chain data tend to confront the researcher with puzzling ambiguity.

Consider once again the integrable $s=1/2$ XY model (3.1) with $h=\gamma=0$. The addition of a Zeeman term $-h_x\sum_l S_l^x$ reflecting the presence of a magnetic field along the x-axis makes the model nonintegrable. The susceptibility $\chi_{xx}(q)$ at $T=0$ and $h_x=0$ thus represents the linear response of the system to a perturbation which renders it nonintegrable. Therefore, any direct determination of $\chi_{xx}(q)$ faces the unfamiliar pitfalls of nonintegrability and cannot be carried out rigorously. However, there is an indirect way to determine this susceptibility exactly: in terms of time-dependent correlation functions of the unperturbed (integrable) model via Kubo's formula

[28]:

$$\chi_{xx}(q) = \frac{1}{2}\sum_{n=-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}qn} \int_0^{\beta/2} d\tau \langle S_l^x(-\mathrm{i}\tau) S_{l+n}^x \rangle. \tag{6.2}$$

For $T = 0$ $\beta \to \infty$), the time-dependent correlation functions entering this expression are exactly the ones portrayed in Sect. 5 except for the difference that the analysis has to be carried out for negative imaginary times. By this method, $\chi_{xx}(q)$ was determined with very high precision [28]. Here we quote the value for $q = \pi$:

$$J\chi_{xx}(\pi) = 0.075566 \pm 0.000005. \tag{6.3}$$

In the present context, it is most instructive to compare this exact result with the results of two numerical methods which have been employed to calculate $\chi_{xx}(\pi)$ by the direct approach, which is susceptible to nonintegrability effects. One method [29] was a $T = 0$ Padé analysis of exact results for $\chi_{xx}^{(N)}(q)$ for finite chains with up to $N = 10$ spins, which yielded the extrapolated value $\chi_{xx}(\pi) \simeq 0.055$. An alternative method [30] based on extrapolations of $T > 0$ calculations of $\chi_{xx}^{(N)}(q)$ for $N = 2, \ldots, 10$ yielded the very different value $\chi_{xx}^{(\infty)}(\pi) \simeq 0.117$. The unreliability of these numerical methods is unprecedented in its extent and most puzzling in the light of previous studies of the same nature on integrable models.

Finally, consider the 1D $s = 1$ generalized bilinear- biquadratic model

$$H = J\sum_{l=1}^{N} \Big[\cos\Theta\, \mathbf{S}_l \cdot \mathbf{S}_{l+1} + \sin\Theta\big(\mathbf{S}_l \cdot \mathbf{S}_{l+1}\big)^2\Big], \quad -\pi/2 \le \Theta \le \pi/2. \tag{6.4}$$

This model is believed to be nonintegrable except forthe two cases $\Theta = -\pi/2$ and $\Theta = \pi/2$, which are amenable to the Bethe ansatz [31].

For the regime $-\pi/2 \le \Theta \le -\pi/4$, Affleck's [32] calculation based on techniques of conformal invariance predicted the presence of an excitation gap which goes to zero continuously in the limit $\Theta = -\pi/2$. This prediction was examined and confirmed by finite-chain studies, which all indicated for $\Theta \neq -\pi/4$ the existence of a gap between the singlet ground state and the lowest triplet excitation [33, 34]. However, more detailed finite-size studies [35] have subsequently revealed the presence of singlet excitations which extrapolate to zero over the entire regime $-\pi/2 \le \Theta \le -\pi/4$, even though they are not the lowest excitations in finite-chains of manageable lengths over at least part of the regime $-\pi/2 \le \Theta \le -\pi/4$. Here we have a situation in which not even the nature of the lowest excitations can reliably be identified unless the spectrum is scrutinized in detail and for relatively large systems [36]. This makes finite-size studies very vulnerable to misleading conclusions if care is not taken. No such phenomenon has ever been observed in exactly solved models.

A similar phenomenon seems to make its appearance in the limit $\Theta = 0$ of this model, which represents the spin-1 Heisenberg AFM (2.3). The excitation gap of this model, first predicted by Haldane [1] on the basis of continuum models, was investigated by finite-chain studies. These studies [37] have produced reasonable evidence that there is indeed a gap of size $\Delta E/J \simeq 0.41$ between the singlet ground state (with wave number $k = 0$) and the lowest finite-chain excitation, which is a triplet state with $k = \pi$. Again, a closer look at the excitation spectrum reveals an unusual class of states to become prominent for $N \ge 12$ [38]. The lowest member of this class is a triplet state with$k = \pi - 2\pi/N$, and extrapolates significantly below the value of the excitation gap ΔE quoted above. A peculiarity of these states is that they do not seem to be members of excitation continua. Nevertheless, they have the potential for upsetting the accepted phase diagram and, therefore, should receive further investigation [36, 38]. Again, there is no precedent for this phenomenon in exactly solved models.

Acknowledgment: This work was supported by a grant from Research Corporation and by the U.S. National Science Foundation, Grant No. DMR-86-03036. The author has greatly benefited from joint projects with J.C. Bonner, R.E. Shrock and J.H. Taylor, the results of which are the backbone of this paper. He is especially indebted to his teacher Harry Thomas, in honor of whose 60th birthday this paper has been presented, for a multitude of reasons, including a series of collaborative endeavors over a full decade, and in particular for his perpetual readiness to offer help, advice and encouragement in scientific matters and beyond. I have used a modified cmpj.sty style file.

References

1. Haldane, F.D.M.: Phys. Lett. **93A**, 464 (1983); Phys. Rev. Lett. **50**, 1153 (1983); (unpublished).
2. Steiner, M., Villain, J., Windsor, C.G.: Adv. Phys. **25**, 87 (1976).
3. *Magnetostructural correlations in exchange coupled systems.* Willett, R.D., Gatteschi, D., Kahn, O. (eds.). Boston: D. Reidel Publishing Co. 1985.
4. Groen, J.P., Klaassen, T.O., Poulis, N.J., Müller, G., Thomas, H., Beck, H.: Phys. Rev. B **22**, 5369 (1980).
5. Anderson, P.W.: Science **235**, 1196 (1987).
6. More precisely: normal modes of the classical equations of motion linearized about the exact classical ground state.
7. Luther, A., Peschel, I.: Phys. Rev. B **12**, 3908 (1975).
8. Müller, G., Thomas, H., Beck, H., Bonner, J.C.: Phys. Rev. B **24**, 1429 (1981).
9. Müller, G., Thomas, H., Puga, M.W., Beck, H.: J. Phys. C **14**, 3399 (1981).
10. Müller, G.: Phys. Rev. B **26**, 1311 (1982).
11. Kurmann, J., Thomas, H., Müller, G.: Physica **112A**, 235 (1982).
12. Taylor, J.H., Müller, G.: Phys. Rev. B **28**, 1529 (1983).
13. Müller, G., Shrock, R.E.: Phys. Rev. B **32**, 5845 (1985).
14. Barouch, E., McCoy, B.M.: Phys. Rev. A **3**, 786 (1971).
15. Suzuki, M.: Prog. Theor. Phys. **46**, 1337 (1971).
16. Yang, C.N.: Phys. Rev. **85**, 808 (1952).
17. Lieb, E., Schultz, T., Mattis, D.: Ann. Phys. (NY) **16**, 407 (1961).
18. Katsura, S.: Phys. Rev. **127**, 1508 (1962).
19. Niemeijer, T.: Physica **36**, 377 (1967).
20. Katsura, S., Horiguchi, T., Suzuki, M.: Physica **46**, 67 (1970).
21. McCoy, B.M., Barouch, E., Abraham, D.B.: Phys. Rev. A **4**, 2331 (1971).
22. McCoy, B.M., Perk, J.H.H., Shrock, R.E.: Nucl. Phys. **B220** [FS8], 35 (1983); **B220** [FS8], 269 (1983).
23. Müller, G., Shrock, R.E.: Phys. Rev. B **29**, 288 (1984); J. Appl. Phys. **55**, 1874 (1984).
24. Lichtenberg, A.J., Lieberman, M.A.: *Regular and stochastic motion.* Berlin, Heidelberg, New York: Springer 1983.
25. Müller, G. : Phys. Rev. A **34**, 3345 (1986).
26. Magyari, E., Thomas, H., Weber, R., Kaufman, C., Müller, G.: Z. Phys. B Condensed Matter **65**, 363 (1987); Srivastava, N., Kaufman, C., Müller, G., Magyari, E., Weber, R., Thomas, H.: J. Appl. Phys. **61**, 4438 (1987).
27. Zaslavsky, G.M.: *Chaos in dynamic systems.* New York: Harwood, 1985.
28. Müller, G., Shrock, R.E.: Phys. Rev. B **30**, 5254 (1984); B **31**, 637 (1985).
29. Duxbury, P.M., Oitmaa, J., Barber, M.N., Bilt, A. van der Joung, K.O., Carlin, R.L.: Phys. Rev. B **24**, 5149 (1981).
30. Bonner, J.C.: p. 157 of Ref. 3.
31. Sutherland, B.: Phys. Rev. B **12**, 3795 (1975); Takhtajan, L.A.: Phys. Lett. **87A**, 479 (1982); Babujian, H.M.: ibid. **90A,** 479 (1982).
32. Affleck, I.: Nucl. Phys. **B265** [FS 15], 409 (1986).
33. Oitmaa, J., Parkinson, J.B., Bonner, J.C.: J. Phys. C **19**, L595 (1986).
34. Blöte, H.W.J., Capel, H.: Physica A (in press).
35. Bonner, J.C., Parkinson, J.B., Oitmaa, J., Blöte, H.W.J. : J. Appl. Phys. **61**, 4432 (1987).
36. Müller, G., Bonner, J.C., Parkinson, J.B.: J. Appl. Phys. **61**, 3950 (1987).
37. Nightingale, M.P., Blöte, H.W.J.: Phys. Rev. B **33**, 659 (1986).
38. Bonner, J.C., Parkinson, J.B.: J. Phys. C (submitted for publication).